Improving Monte Carlo and Molecular Dynamics Simulation Outcomes Using Temperature-Dependent Interaction Parameters

Ali Al-Matar [C, S], Ahmed Tobgy, Ibrahim Suleiman and Majdi Al-Faiad
University of Jordan, Chemical Engineering Department, Amman, Jordan
aalmatar@ju.edu.jo

The main proposition of this work is that introducing temperature-dependent interaction parameters (TDIP) instead of the current practice of using temperature-independent interaction parameters (TIIP) may lead to improvement in the prediction of phase equilibrium properties such as VLE, and transport properties e.g., self-diffusivity. Published second virial coefficient data was used to fit several simple two parameter temperature dependent models for the collision diameter and well depth. This fitting procedure reduce the RMSD between the experimental and the predicted second virial coefficient by tenfold compared to the best temperature independent parameters obtained in this research and by fifteen fold with the literature values. The vapor-liquid coexistence curve for argon was simulated in the NVT Gibbs ensemble (GE) using the Monte Carlo (MC) technique developed by Panagiotpoulos (1987). The simulations were carried out using both TDIP and TIIP in the temperature range: 110–148 K. The critical temperature and density were determined using the Ising-scaling model. The TDIP simulations produce, in general, a more accurate phase diagram compared to the diagram generated using TIIP. The RMSD is reduced by 42.1% using TDIP. Also, there was no significant difference between the results obtained using TDIP and the highly accurate and computationally demanding phase diagrams based on three body contributions. Self-diffusivities of atomic argon were evaluated by means of the mean square displacement or the Einstein method using equilibrium molecular dynamics (MD) at a pressure of 13 bar and a temperature range from 90 K up to 135 K in the isobaric, isothermal NPT ensemble. TDIP, in general, produces more accurate self-diffusivities than the values computed by TIIP simulations. Comparing the two approaches, the relative percentage error is reduced by about 67% and the RMSD is reduced by about 64% by using the temperature-dependent parameters.